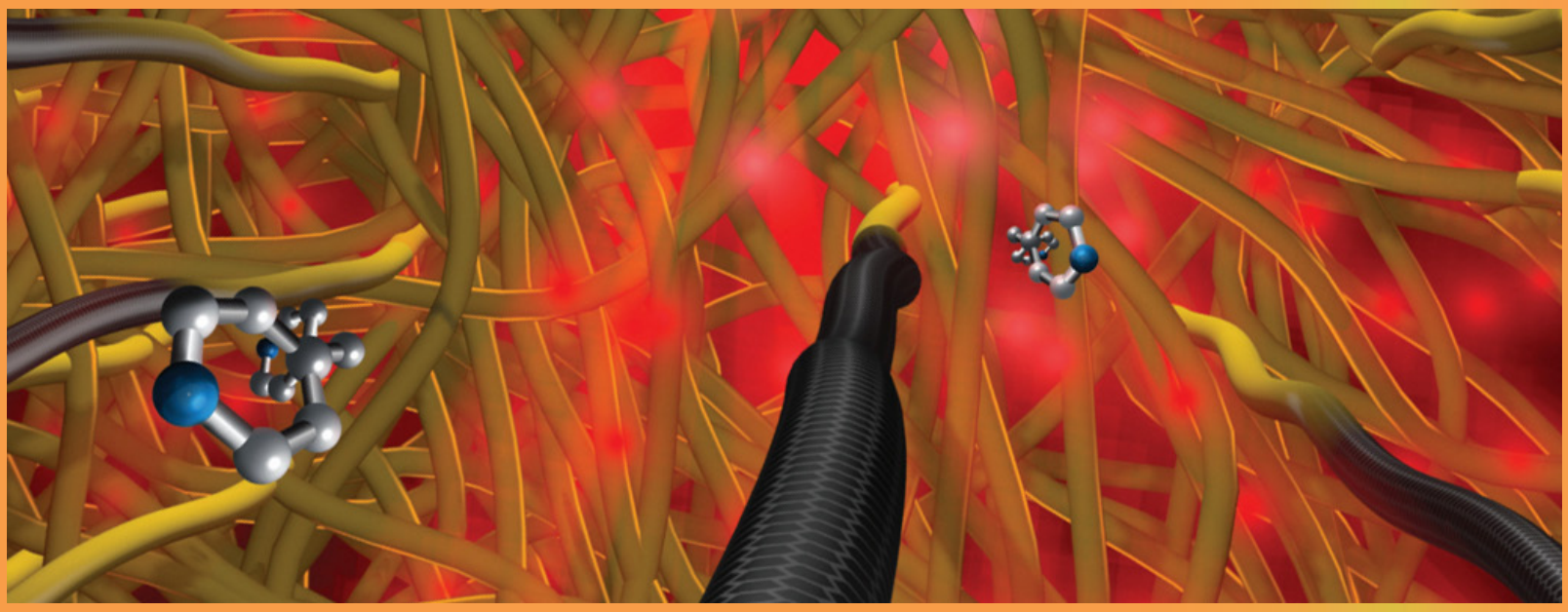
Science and Technology UPDATE

September/October 2013

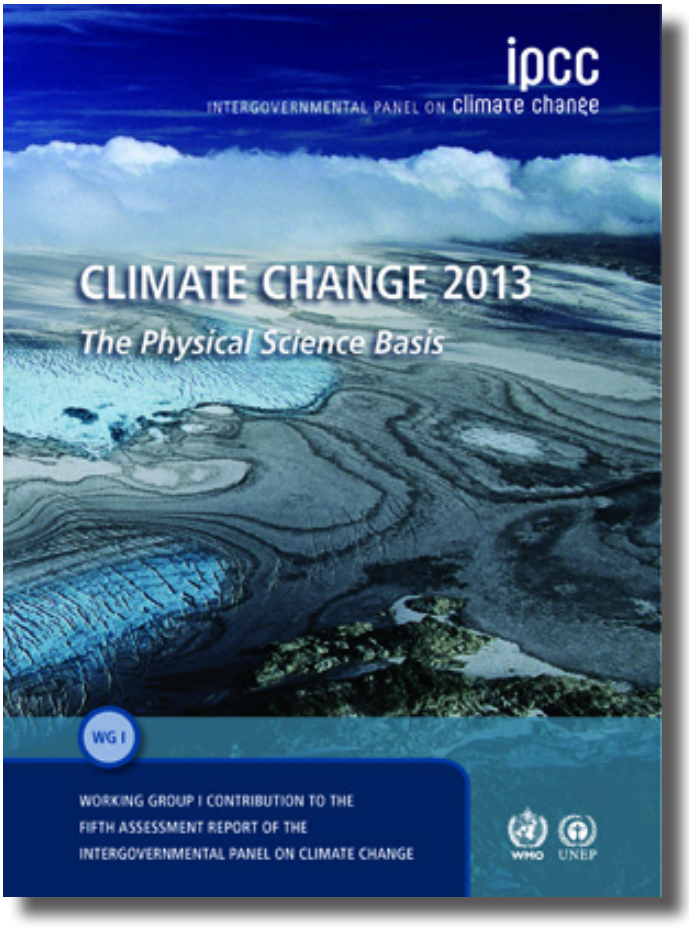


Science on a Mission

LLNL-MI-645596

LIVERMORE SCIENTISTS PLAY KEY ROLES IN 5TH CLIMATE REPORT

Over the past 3 years, Laboratory scientists have made significant contributions to the ***5th Assessment Report*** by the Intergovernmental Panel on Climate Change. Phil Duffy was part of a six-person team representing the U.S. in final negotiations for the report's "**Summary for Policy Makers**," which for the next 6 or 7 years will be the most definitive statement available about recent climate change and will be the basis for climate policy, including international negotiations to limit future greenhouse gas emissions and any discussions of compensation for damages from past emissions. Most of the climate-modeling research assessed in the *5th Assessment Report* is based on results made by the LLNL's Program for Climate Model Diagnosis and Intercomparison through the LLNL-led **Earth System Grid Federation**. Other Laboratory staff contributing to the text of the *5th Assessment Report* include Peter Gleckler (a lead author) and Karl Taylor (a review editor).



SCIENTIST HONORED BY NATO FOR DISCOVERY OF ENERGETIC MOLECULE

Phil Pagoria received the 2013 NATO Munitions Safety Award for Technical Achievement in recognition of his discovery and development of the energetic molecule LLM-105, which has potential applications in enhancing the safety of nuclear and conventional weapons. Phil called the award "a testament to the employees (past and present) of the LLNL Energetic Materials Center, the LLNL High-Explosives Application Facility, and the S300 B827 pilot plant." He was nominated for the award by the U.S. Army and the Office of the Secretary of Defense/Acquisition, Technology, and Logistics. Phil's work over the years was supported by the LDRD Program through multiple projects.

SCINTILLATOR LICENSED FOR RADIATION DETECTION

Livermore technology for solution-grown organic scintillators has been licensed for the field of radiation detection. The licensee plans to utilize the rights granted under this license to manufacture and sell initially two product types: packaged stilbene and assemblies with integrated light-sensing devices. The company intends to target applications in homeland security and treaty compliance, including nonproliferation.

About the Cover

An illustration of the "kissing nanowire" effect, in which a laser induces local plasmonic enhancement of the electromagnetic field at carbon nanotube junctions. (See "SERS combined with nanowires . . ." on pg. 13.)

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-7NA27344.

NEURAL TECHNOLOGY ENGINEERS PRESENT AT BIOSCIENCE CONFERENCE

Neural technology engineers Kedar Shah and Vanessa Tolosa recently gave presentations at the **35th Annual International Conference** of the IEEE Engineering in Medicine and Biology Society held in Osaka, Japan. Both engineers presented on their work in LLNL's **Center of Micro and Nano Technology** to develop medical devices for enhancing basic human functions such as eyesight, hearing, and speech. The presentations helped raise awareness of the Lab's research in a field where, only 2 years ago, many were unaware of LLNL's work on neural interfaces. Both presenters, however, attest to a dramatic increase in Livermore's visibility. "Now," says Vanessa, "we are getting people coming to our talks and posters, fully aware of what we do and coming to find out our progress in the field." In the photo, Vanessa holds up a finished silicon wafer on which polymer neural interfaces are fabricated.

DoD ANNOUNCES SUCCESSFUL SLED TEST OF LLNL-DESIGNED CONVENTIONAL WARHEAD

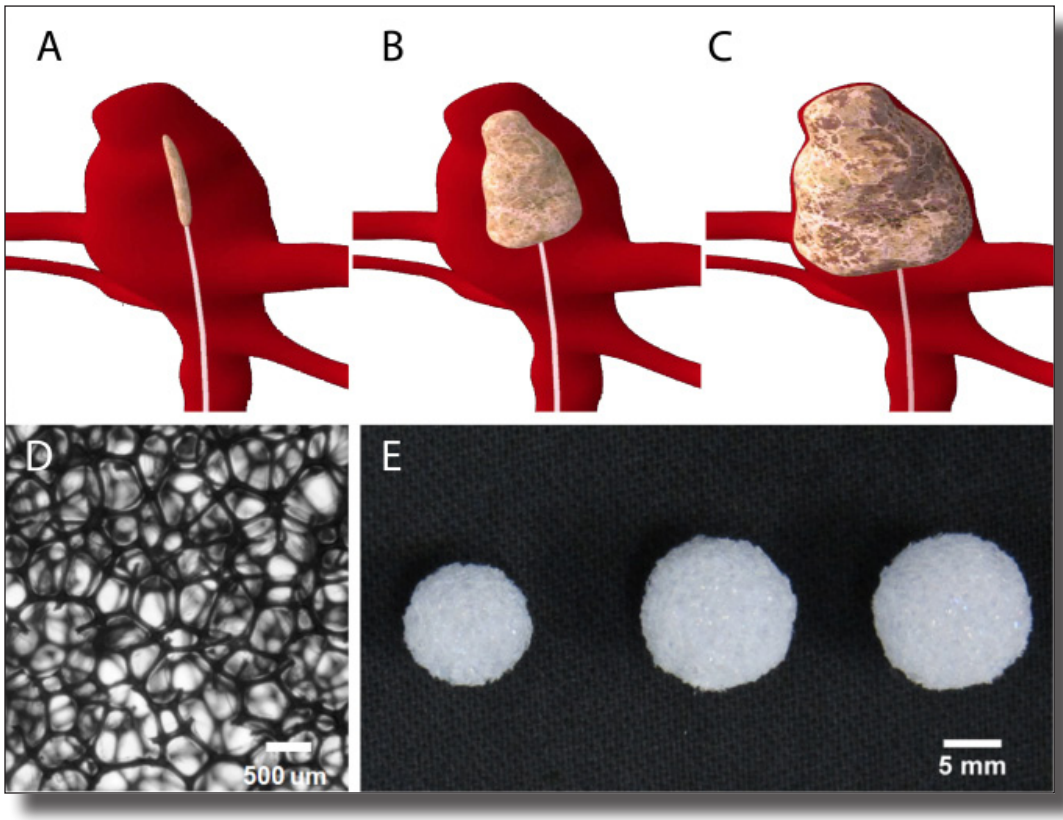
The Department of Defense announced the successful "sled test" of an advanced conventional warhead designed by LLNL under the Conventional Prompt Global Strike Initiative. The warhead, a kinetic-energy projectile also known as a precision effects warhead, is being developed as a central part of a larger effort to establish the capability to deliver a conventional projectile at hypersonic speeds and with great precision. The successful test "demonstrated that the warhead functions in a flight-representative environment," said a DoD representative, bringing the program "one important step closer" to its ultimate objective. The Laboratory served as technical lead and integrator of this testing at Holloman Air Force Base, which was meant to simulate the dynamic environment in which the warhead will operate and which follows computer simulation and, more recently, monorail hypersonic testing of the sled itself.

AWARD FOR CONTRIBUTORS TO SPECIAL NATIONAL INTELLIGENCE ESTIMATE

As part of a multiagency team tasked with contributing to a Special National Intelligence Estimate (SNIE), Chris Carson received an Intelligence Integration Award from the Office of the Director of National Intelligence. The team also included Debbie Andrews, Frank Daffin, Larry Logory, and Roger Miller, as well as DOE employees Heather Crockett and Mike McKeon. The entire team was recognized "for its demonstrated professional integrity, enthusiasm, and dedication to producing a SNIE on a sensitive [weapons of mass destruction] topic, demonstrating deep substantive knowledge, great sensitivity to alternative analysis, and the highest standards of analytical tradecraft." The award noted that the SNIE has had "a direct impact on foreign policy and national security."

SHAPE MEMORY FOAMS FOR TREATING ANEURYSMS CLOSER TO CLINICAL TRIALS

Texas A&M University **announced** that polyurethane-based shape memory polymer foams originally developed at LLNL are one step closer to clinical trials as a treatment for aneurysms after demonstrating their ability to promote "healing at unprecedented levels." The foams, first developed by a team including LLNL's Thomas Wilson and then-LLNL researcher Duncan Maitland, are biocompatible materials used to fill the aneurysm vein pouch, which can cause death if it ruptures. As recently **announced in a paper** in the *Journal of Biomedical Materials Research Part A*, the foams are an alternative to the current approach of using a platinum coil, which poses its own health risks, such as inflammation that impedes healing or compaction over time that can lead to rupture. Before placement, a shape memory foam is formed into a primary shape that fits the aneurysm, crimped into a smaller, temporary shape that enables placement, and then expanded back to their primary state by an increase in temperature. The figure shows (a–c) illustrations of a crimped shape-memory foam device inserted into an aneurysm and expanded to its permanent shape; (d) a closeup of the foam lattice; and (e) actual foam devices in their pre-crimped shapes.



BIOAMS ACHIEVEMENTS HIGHLIGHTED IN *PHYSICS TODAY*

An "Issues and Events" article in *Physics Today* **highlights some of the Laboratory's pioneering efforts** in using accelerator mass spectrometry (AMS) to address challenges at the forefront of biology and biomedical science. The article covers a recent application of microdosing and its application to understanding how people metabolize a promising new cancer drug. Microdosing involves giving small, subtherapeutic amounts of a drug that are unlikely to produce whole-body effects but that are high enough to study how the drug is taken up in the body and metabolized. The exquisite sensitivity of AMS enables the investigation of the pharmacokinetics of carbon-14-labeled drugs administered at almost negligible levels. The article also highlights the recent finding, based on bomb-pulse dating of brain tissue, that at least parts of the human brain continue to form new neurons throughout one's life, contrary to longstanding conventional wisdom. Finally, the article covers recent LDRD-funded work at Livermore's Center for Accelerator Mass Spectrometry to develop an optical spectroscopic technique for measuring carbon isotope ratios, a technique that is potentially far simpler and cheaper than AMS and that would make the use of carbon-14 tracers far more accessible to medical and biological researchers.

RESEARCHER TO CHAIR COMMITTEE ON PASSENGER-SCREENING X-RAY MACHINES

Harry Martz, head of the Laboratory's **Center for Nondestructive Characterization**, has been asked to chair the Committee on Airport Passenger Screening: Backscatter X-Ray Machines. Sponsored by the National Research Council, **the committee** has more than a dozen members representing numerous prestigious academic and medical institutions and industry, including Columbia University Medical Center, Harvard Medical School, the University of Illinois, and BAE Systems. Commissioned by the **Explosives Division** of the Homeland Security Advanced Research Projects Agency, the committee will review previous studies and current processes used by the Department of Homeland Security and equipment manufacturers to estimate radiation exposure from backscatter x-ray imaging systems used to screen air travelers. The committee will then report its findings and recommendations concerning compliance with health and safety standards and the prevention of overexposure to ionizing radiation. The photo shows Harry checking a case about to be inserted into an explosive detection system to obtain x-ray signature data on the case's contents.

RESEARCHER WINS 2013 EDWARD TELLER AWARD

On August 20, the American Nuclear Society (ANS) announced the recognition of Livermore's Jim Hammer as one of two recipients of the 2013 Edward Teller Award. Jim, who is also one of the Laboratory's Distinguished Member of Technical Staff, is co-inventor of the fast-ignition approach to nuclear fusion energy. The Edward Teller Award recognizes pioneering research and leadership in the use of laser and ion-particle beams to produce unique, high-temperature and high-density matter for scientific research and for controlled thermonuclear fusion. Through its honors and awards program, ANS recognizes the exceptional accomplishments of nuclear science and technology professionals.

TWO APS FELLOWS ELECTED

John Moody and Pravesh Patel were elected fellows of the American Physical Society (APS) after being recommended by the APS Division of Plasma Physics. John was recognized for his "pioneering experiments contributing to understanding propagation, scattering, transmission, and redirection of high-intensity laser beams in large-scale plasmas for inertial confinement fusion." Pravesh was recognized for his "pioneering contributions in the science of ultra-intense laser–matter interaction and particle acceleration and applications to creating and probing high-energy-density plasma states, and for his leadership in advancing the fast ignition concept for inertial confinement fusion."

SCIENTIST INTERVIEWED BY CNN ON SYRIAN CHEMICAL WEAPONS INVESTIGATION

Hugh Gregg, who is currently on government service leave from LLNL to serve as head of the Laboratory of the Organisation for the Prohibition of Chemical Weapons (**OPCW**) in The Hague, Netherlands, was recently **interviewed by CNN** about the work that the OPCW in general—and his laboratory specifically—did to support the investigation into the use of chemical weapons in Syria. The OPCW is the implementing body of the Chemical Weapons Convention, an international treaty that bans the possession of chemical weapons and that has been signed and ratified by 189 countries around the world.

SEISMOLOGIST INTERVIEWED BY NATIONAL MEDIA ON NEW ISLAND APPEARING AFTER QUAKE

Laboratory seismologist Robert Mellors, an expert on mud volcanoes, was interviewed on September 24 **by the Weather Channel** and then the next day **by ABC News** as part of the news outlets' reporting on the appearance of a new island offshore of the Arabian Sea port of Gwadar following a magnitude-7.7 earthquake in Pakistan. The new island is likely a mud volcano formed by the earthquake-triggered release of methane and other gasses that had been trapped in subsea sediments. "There is nothing exceptionally unique about this one," said Robert, "other than it was triggered by a far away earthquake directly, which is rare." Being comprised primarily of mud, the island is not expected to remain above the sea surface for very long.

LISA POYNEER TO SERVE ON NASA TECHNOLOGY ANALYSIS COMMITTEE

Lisa Poyneer has been selected to serve on the NASA Technology Analysis Committee in support of development of the Astrophysics Focused Telescope Assets–Wide-Field Infrared Survey Telescope (**AFTA–WFIRST**) mission concept. The mission combines the AFTA design on an existing 2.4-meter telescope with the main instrument, a wide-field, near-infrared imager for studying dark energy. It also has a coronagraph instrument for directly imaging exoplanets and debris disks. The primary responsibility of the committee will be to assess the technology readiness of AFTA mission-critical technologies and to provide NASA with analyses for the planning of future technology development.

"HIGH-FOOT" NIF SHOT TREBLES RECORD FOR NEUTRON YIELD

A NIF shot on August 13 directed all 192 beams at a deuterium–tritium target, which released a neutron yield of nearly 3×10^{15}, or approximately 8,000 joules of neutron energy—approximately three times NIF's previous neutron yield record for cryogenic implosions. Part of the "high foot" campaign, this experiment was designed to increase the target shell's resistance to performance-degrading breakup by increasing laser power during the "picket" (first two nanoseconds) of the laser pulse, resulting in a pulse with a higher temperature in its trough (also known as the "foot" of the pulse, hence the term high-foot pulse). This latest NIF accomplishment provides an important benchmark for the program's computer simulation tools and represents a step along the "**path forward**" to ignition delivered to Congress in December 2012. Attaining conditions not observed since the days of underground nuclear weapons testing, the experiment also represents an important milestone in the Laboratory's stockpile stewardship mission.

AT LVOC, A DAY FOR POTENTIAL TARGET FABRICATORS

On September 11, NNSA hosted a Target Fabrication Industry Day at the Livermore Valley Open Campus as part of efforts to recruit manufacturers capable of supporting the fabrication of targets for the National Ignition Facility (NIF). At the event, participants heard explanations of the inertial confinement fusion and high-energy-density research programs and the industrial capabilities required to manufacture targets for NIF. In the photo, LLNL target fabrication manager Alex Hamza explains current technical requirements and anticipated future technical needs for NIF targets.

LLNL HOSTS MESOSCALE MATERIALS SCIENCE WORKSHOP

On August 13–15, the Laboratory held a workshop on **mesoscale materials science** that was attended by 115 external and internal participants. The workshop's goal was to identify priority research direc-

tions for mesoscale materials science, to identify potential new collaborators for the Lab, and to prepare for potential new funding opportunities in this area. The workshop focused on four themes: super-grain structures and collective microstructural phenomena, defect interactions from dislocations to grains, directed assemblies and collective phenomena at the mesoscale, and mesoscale architectures in advanced manufacturing. The workshop featured plenary lectures by notable experts from academia and industry, was funded by the Lab's Office of Strategic Outcomes, and was planned entirely by LLNL staff members—Young Han, Mukul Kumar, Christian Mailhiot (now at Washington State), Robert Rudd, Chris Spadaccini, Eric Schwegler, and Tony van Buuren.

PARTNERING TO COMMERCIALIZE TREATMENT FOR DEAFNESS

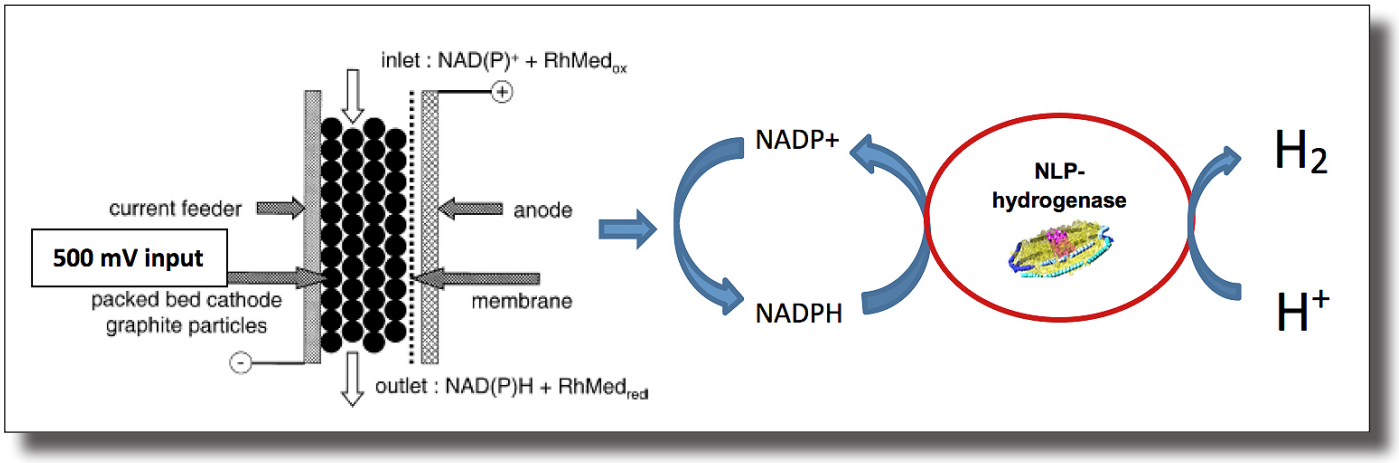
The Laboratory has received phase 1 funding to develop a wireless power telemetry system in collaboration with Bay Area startup **OtoKinetics**, which seeks to commercialize a technology to treat deafness with better performance than is possible with current cochlear implants. The new approach differs from current technologies by using a piezoelectric microactuator that produces sound waves in the fluid of the cochlea, which are then transmitted into the brain, much like normal hearing. The power telemetry system will enable the device to be powered wirelessly, removing the need for implanted batteries or electrical wires penetrating through the skin. In this partnership, LLNL is applying its expertise in biocompatible materials and their implantation processes that were developed under the **Artificial Retina Project** and other neural prosthetic efforts.

USE OF LASER PEENING IN JET-ENGINE MANUFACTURING CONTINUES TO EXPAND

Use of laser peening technology originally developed at LLNL **is being expanded** at a Rolls-Royce manufacturing plant, according to LLNL licensee Curtiss-Wright. The technique, which reduces metal fatigue, is being used in a laser peening production cell that **Curtiss-Wright built and now operates** to process "wide chord" fan blades for Rolls-Royce's "Trent" aero engines.

NANOLIPOPROTEIN TECHNOLOGY OPTIONED FOR HYDROGEN PRODUCTION

The Laboratory recently optioned LLNL nanolipoprotein (NLP) technology with possible application in hydrogen production for energy applications. The technology was optioned by Nzyme2HC, LLC, which now has an exclusive, time-limited right to negotiate a license agreement in the specific field of use. The image gives an overview of the process of ex vivo hydrogen production using molecular constructs consisting of NLP and the enzyme hydrogenase.

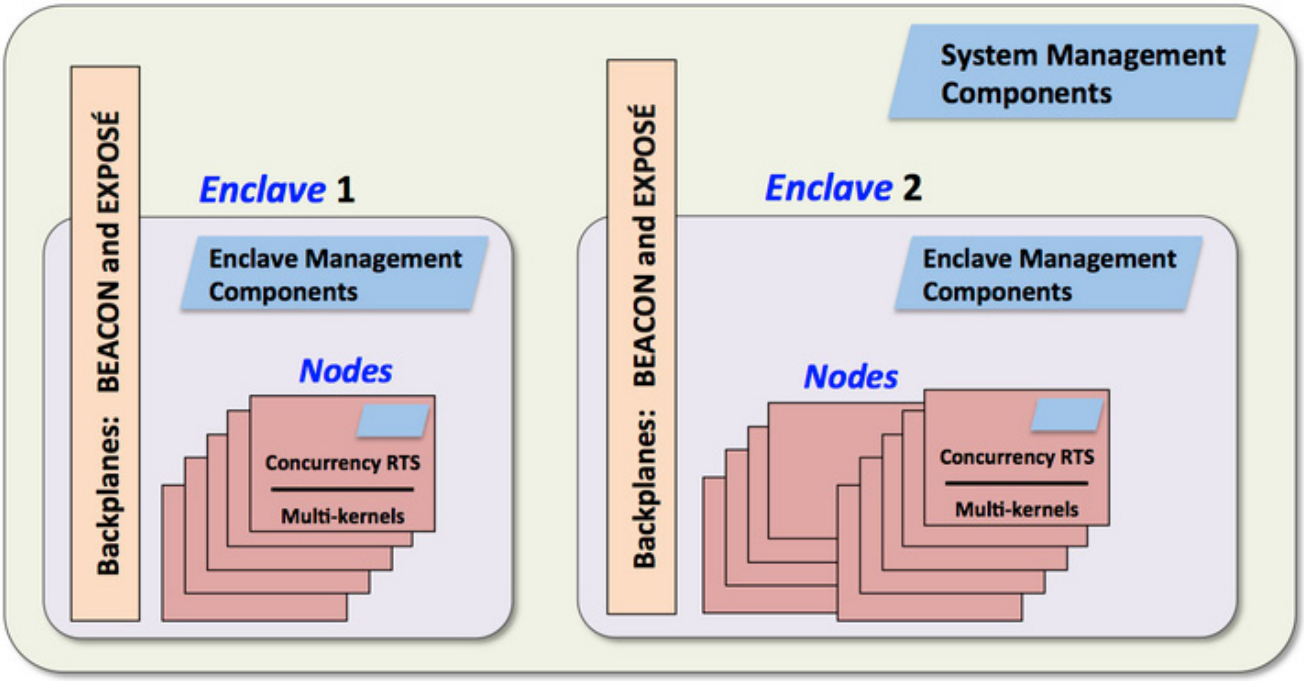


MULTI-INSTITUTIONAL EXASCALE ARCHITECTURE PROJECT FUNDED

A three-year, $9.75 million project—named Argo—to design and develop a platform-neutral prototype of an exascale operating system and runtime software has been funded by the Office of Science. Lead institution Argonne National Laboratory will collaborate with LLNL—where the point of contact is Maya Gokhale—along with Pacific Northwest National Laboratory and several universities. At the heart of Argo are four key innovations: dynamic reconfiguring of node resources in response to workload, allowance for massive concurrency, a hierarchical framework for power and fault management, and a "beacon" mechanism for communicating with and controlling the platform. These innovations will result in an open-source prototype system that runs on several architectures. Argo is expected to form the basis of production exascale systems deployed in the 2018–2020 timeframe. The figure is an architecture overview of Argo.

RESEARCH ON ANTHRAX PRESENTED AT INTERNATIONAL CONFERENCE

Livermore researchers contributed significantly to **Bacillus ACT 2013**, an international conference that brings together the world's specialists on *Bacillus anthracis*—which causes anthrax—and two closely related bacilli, *B. cereus* and *B. thuringiensis*. This year's conference, held September 1–5 in Victoria, Canada, was co-chaired by LLNL's Paul Jackson, who also chaired one of the conference's sessions. Of the 65 technical talks, four were given by LLNL researchers—Crystal Jaing, Feliza Bourguet, Alexis Dunkle, and Stacy Kane. Several of the 105 posters presented were also from LLNL. The primary mission of the Bacillus ACT conferences is to promote interactions among investigators researching the physiology, genetics, molecular biology, pathogenesis, and ecology of these three closely related bacteria and their kin.



GRANT FOR RESEARCH ON CLIMATE–MARINE MICROBIOLOGY LINK

Xavier Mayali has received a grant of nearly $1 million from the Gordon and Betty Moore Foundation's **Marine Microbiology Initiative** to study how the food preferences of coastal marine microorganisms shape elemental cycles in the ocean. The Foundation's grant, which will be administered through Oregon State University (OSU), will allow Xavier and LLNL colleague Jennifer Pett-Ridge, along with coinvestigators at OSU and Oak Ridge National Laboratory (ORNL), develop a deeper understanding of how the food choices of marine microbes contribute to carbon cycling off of the coast of California. High-precision isotopic techniques and molecular biology methods that are being pioneered at LLNL and ORNL will be used to identify which microbes prefer which general types of organic molecules (e.g., lipids, carbohydrates, proteins, and nucleic acids) and how microbe–foodweb interactions affect the marine carbon cycle. Developing a better understanding how the marine biosphere will respond to increasing levels of atmospheric CO_2 is vitally important for reducing the uncertainty in climate model predictions.

RESEARCHER IN LINE TO CHAIR APS FAR WEST SECTION

Peter Beiersdorfer has been elected to the "chair line" of the American Physical Society's Far West Section (formerly known as the California–Nevada Section). Peter was elected by members of the section. The four-year chair line entails him serving first as vice chair of the section for one year, then in successive years as chair-elect, chair, and finally past chair. Peter, who is currently member-at-large on the Executive Committee, will begin his four-year chair line on January 1, 2014.

LAB CO-SPONSORS ANOMALOUS ABSORPTION CONFERENCE

The 43rd Annual Anomalous Absorption Conference, co-sponsored by LLNL and UC Davis, was held July 7–12. The conference brought together scientists from various fields involved in laser–matter interactions and high-energy-density physics. LLNL's Denise Hinkel delivered welcoming remarks and closing comments, presented the results of recent NIF experiments, and described a new NIF target called the quartraum or quarter-hohlraum—a platform for investigating cross-beam energy transfer (CBET) as laser beams enter the hohlraum. Pierre Michel also discussed CBET, while Laurent Divol described the use of indirect-drive "exploding pusher" targets on NIF. Mordy Rosen discussed how low-density, gas-filled hohlraums provide a platform to study hohlraum physics that is intermediate between gold spheres and ignition hohlraums. Finally, Peter Amendt gave a talk on shock-driven resistive heating in mixed-species thermonuclear fuels. Other LLNL speakers were Ed Williams, Tom Chapman, Jeffrey Banks, John Moody, David Strozzi, Scott Wilks, and Claudio Bellei.

THIRD IZEST MEETING ON ULTRAHIGH-ENERGY LASERS HELD AT LLNL

The **third meeting** of the International Center for Zettawatt-Exawatt Science and Technology Research (IZEST) was held at LLNL on July 17 and 18. This series of international meetings is held in support of IZEST, which works to develop exawatt (quintillion-watt) and zettawatt (sextillion-watt) laser systems. Invited presentations and poster sessions addressed the development and status of novel ultrahigh-energy laser technologies around the world, such as the Exawatt Center for Extreme Light Studies in Russia, the Texas Petawatt Laser, Europe's Extreme Light Infrastructure, and the Petawatt Aquitaine Laser in France. Other talks discussed frontier ultrahigh-intensity science, along with applications that may be pursued with these lasers. A dedicated session looked

at how best to leverage NIF and similar megajoule-class laser systems to produce exawatt-peak-power laser pulses, as well as what high-impact, ultrahigh-intensity experiments might be conducted on such facilities.

DEVELOPING INTERNATIONAL STANDARDS FOR RADIATION DETECTION INSTRUMENTATION

For the past 11 years, nuclear physicist and health physicist Radoslav Radev has been helping develop international standards for radiation detection instrumentation as a member of the Radiation Protection Instrumentation Subcommittee of the Nuclear Instrumentation Technical Committee of the International Electrotechnical Commission (**IEC**). He has contributed to more than a dozen international standards. Most recently, Radoslav served as project leader for developing the highly challenging standard "Neutron Ambient Dose (Rate) Meters" (IEC 61005). After several years in the making, this standard is now being finalized and is expected to be published in 2014. U.S. experts on the IEC subcommittee and committee are drawn from the Department of Homeland Security, U.S. Customs and Border Protection, the National Institute of Standards and Technology, instrument manufacturers, and private consulting groups; Radoslav is one of the few representatives from the DOE complex and the only one from LLNL. Founded in 1906, the IEC is the world's leading organization for preparing and publishing international standards for electrical, electronic, and related technologies, which the IEC does in cooperation with two sister organizations—the International Organization for Standardization and the International Telecommunication Union.

SCIENTIST TO BE PRESIDENT OF MINERALS, METALS, AND MATERIALS SOCIETY

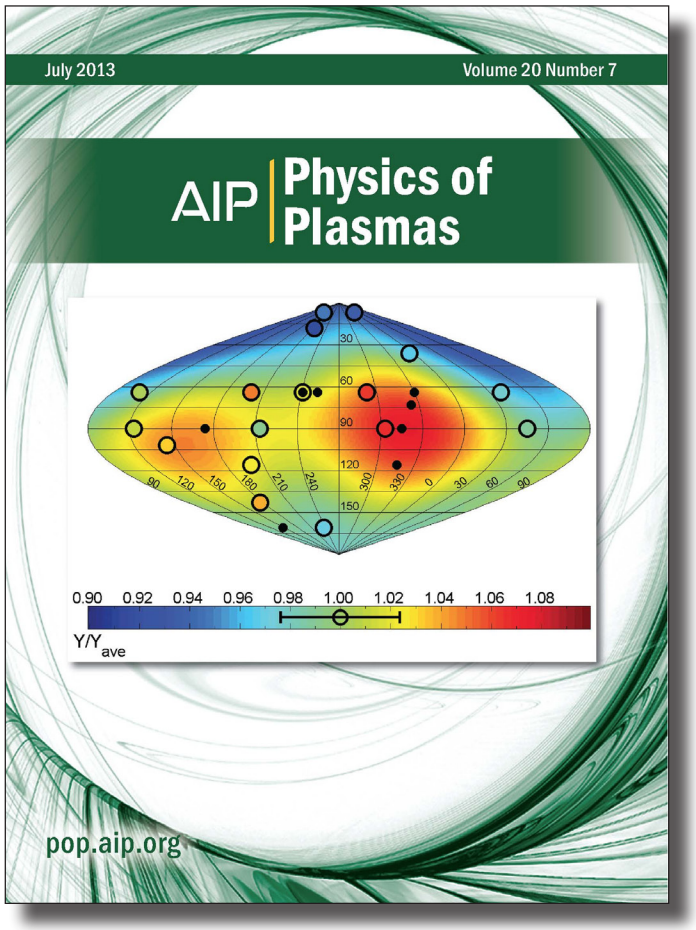
Patrice Turchi has been selected by members of The Minerals, Metals, and Materials Society (TMS) to serve in the society's "presidential cycle." Beginning at the next annual meeting of TMS, in February 2014, Patrice will serve first as TMS vice president, then president, and finally past president. TMS is a member-driven professional society of scientists and engineers working in materials-related fields in industry, academia, and government, along with students in those fields. Included among its nearly 12,000 members are metallurgical and materials engineers, scientists, researchers, educators, and administrators from more than 70 countries on six continents.

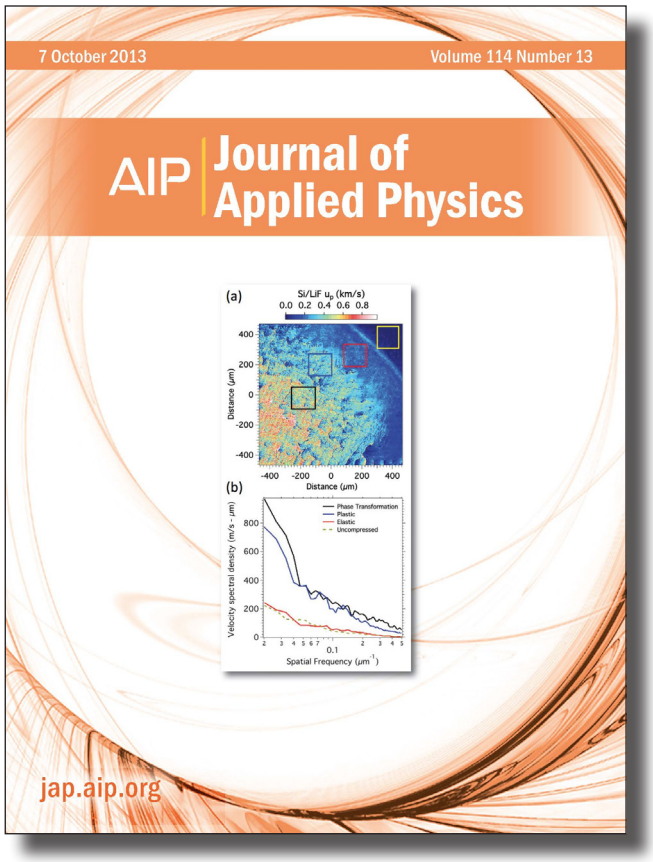
SEXUALLY TRANSMITTED DISEASE DETECTOR OPTIONED

Malignext Target Technologies, Inc. in March licensed Laboratory technology for a disposable panel detector for sexually transmitted diseases. Malignext, a small business located in Vancouver, WA, is also in the research phase of developing a product that will be able to mark or make palpable lesions or tumors of the breast.

NIF IGNITION PROGRESS ON *PHYSICS OF PLASMAS* COVER

The July 2013 issue of *Physics of Plasmas* contains **a review article on progress towards ignition at NIF**, and the cover of that issue features an image of the spatial distribution of primary neutrons from a shot as measured with flange nuclear activation detectors that are distributed around the NIF target chamber. The paper discusses experimental trends, possible causes of degraded performance—that is, discrepancies relative to model predictions—and the plan to understand and resolve the underlying physics issues.



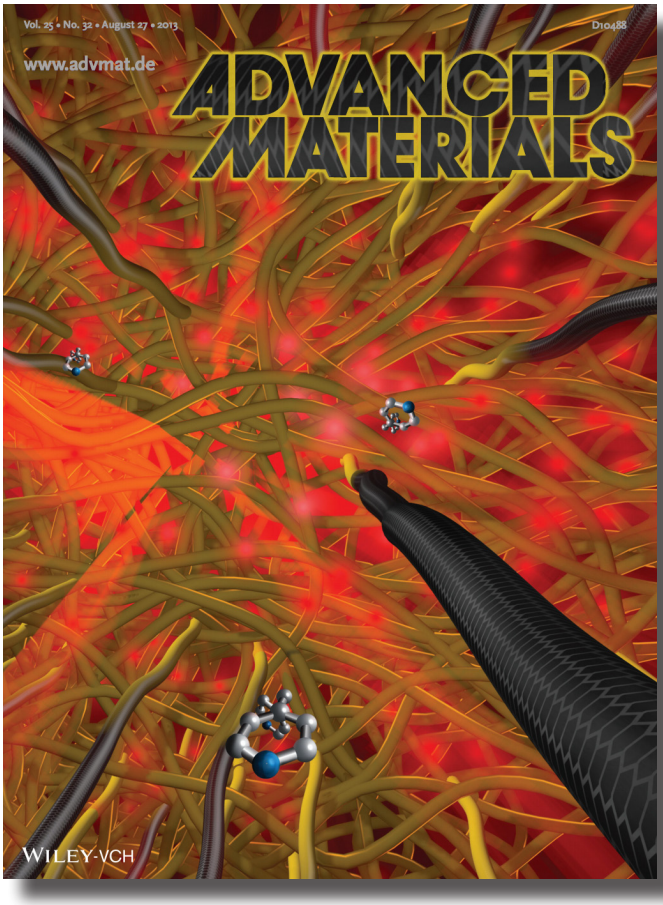


NEW METHOD INVESTIGATES MICROSCALE EVOLUTION OF SHOCKED MATERIALS

In **a paper featured on the cover** of *Journal of Applied Physics*, Ray Smith and colleagues from LLNL, LANL, UC Berkeley, and Princeton describe the use of a recently developed high-resolution, two-dimensional (2D) version of the velocity interferometer system for any reflector (VISAR) combined with 1D VISAR measurements to construct a time-resolved picture of deformation in shock-compressed crystal silicon. The data collected can reveal the rich complexity of heterogeneous flow not recorded by standard velocimetry techniques. In silicon crystal, the team documented variations in particle velocities caused by plastic deformation along preferred planes and a dramatic change in flow as a phase transformation occurred at approximately 13 GPa. Work at LLNL was supported by Livermore's LDRD Program.

SERS COMBINED WITH NANOWIRES COULD ENABLE SINGLE-MOLECULE DETECTION

In a paper featured on the cover of *Advanced Materials*, LLNL's Tiziana Bond and colleagues at Switzerland's Institute of Energy Technology describe **an innovative sensor based on surface-enhanced Raman spectroscopy** (SERS) with which the team was able to detect an organic species in a concentration of a few hundred femtomoles per liter. The team combined SERS with densely packed bundles of carbon nanotubes (CNT) to create "hot spots" where sensitivity was greatly enhanced. To enhance the effect further and make detection more reliable, the end of the nanotubes were coated with hafnium dioxide and then gold, creating thousands of high-density nanometer-sized hot spots within a 3-D structure. By boosting sensitivity by as much as 100,000 times, such CNT-enhanced SERS spectroscopes could approach the goal of single-molecule detection in an inexpensive portable device. This work was supported at LLNL by the LDRD Program.

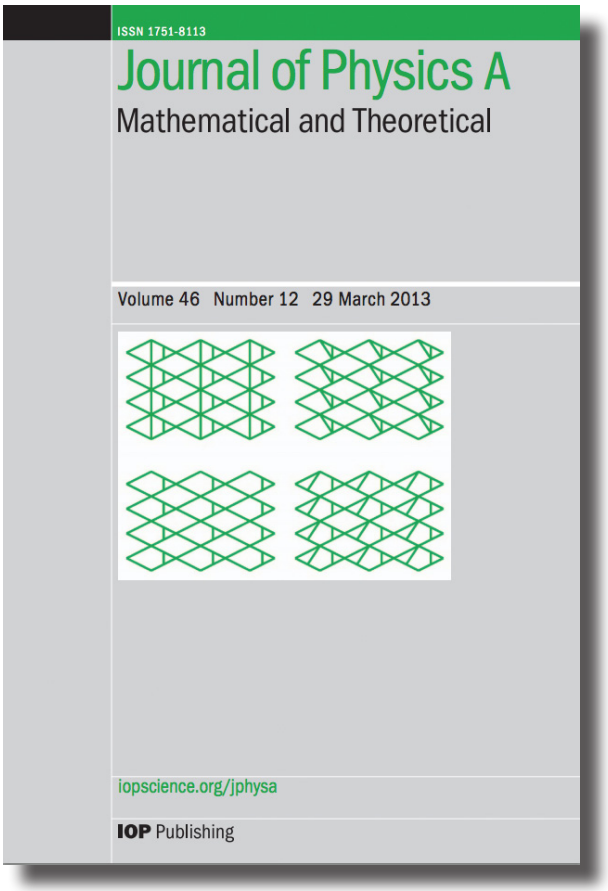


MOLECULAR DOCKING PROGRAM ON JOURNAL COVER

The cover of the April 30, 2013 issue of *Journal of Computational Chemistry* features a paper by LLNL researchers Xiaohua Zhang, Sergio E. Wong, and Felice C. Lightstone **describing a molecular docking program** that the team parallelized for use on future exascale machines. **VinaLC**—"LC" stands for "Livermore Computing"—was tested at LLNL and shown to scale up to more than 15,000 central processing units (CPUs) with a very low overhead costs. In addition to speed—one million flexible compound docking calculations took only 1.4 hours to finish on the 15,000 CPUs—the team also verified the accuracy of their new approach. With computation playing a larger and larger role in the screening of drug candidates, which can now be examined virtually before laboratory testing, proven programs such as VinaLC open the door to far less expensive drug development.

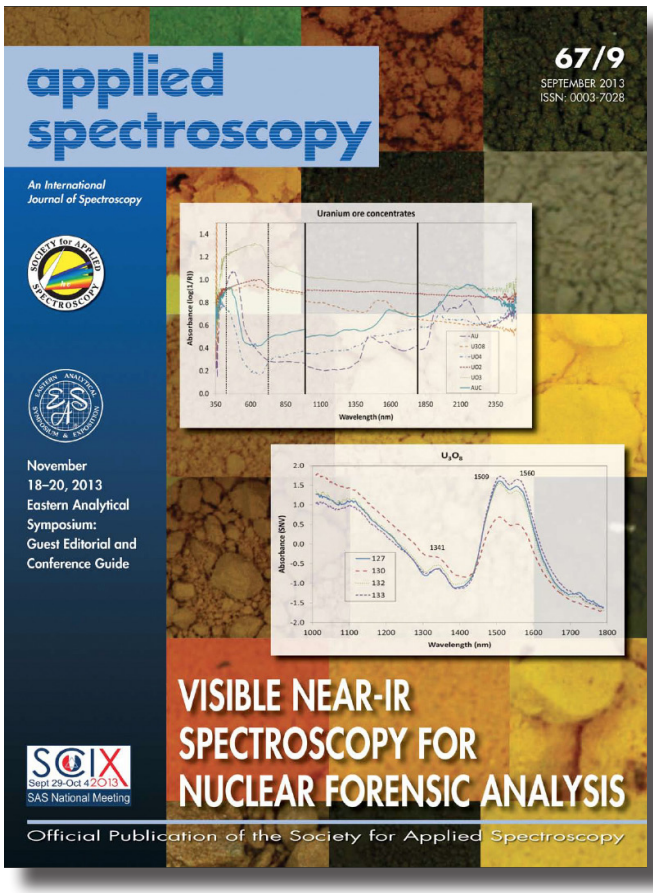
POSTDOC PAPER ON SOLVING TWO-DIMENSIONAL BOW-TIE LATTICES

An article lead-authored by LLNL postdoc Christian Scullard was the cover feature for the March 29 issue of *Journal of Physics A*. The work is on the q-state Potts model, which is an idealized model of ferromagnetism, and involves the critical temperature at which a sharp transition to complete disorder occurs. In two dimensions, there is a narrow class of lattices where exact transition temperatures can be found. The solution for lattices with square cells is believed to be very difficult in general, but this paper describes how a subset of them—such as the "asymmetric bow-tie" lattices that appear on the journal's cover—are solved using a transformation of couplings on triangular cells. Christian worked with a colleague at France's Laboratory of Theoretical Physics—a collaboration stemmed from a chance encounter at a conference at UC Berkeley. "This flexibility is one of the many great things about being a postdoc at LLNL," said Christian.



NUCLEAR FORENSICS WORK ON URANIUM ORE ON COVER OF *APPLIED SPECTROSCOPY*

The cover of an issue of *Applied Spectroscopy* features a paper—authored by Livermore's Gregory Klunder, Jonathan Plaue, Paul Spackman, Patrick Grant, Rachel Lindvall, and Ian Hutcheon—that **describes the application of visible and near-infrared reflectance spectroscopy** to nuclear forensic analysis and attribution involving uranium ore concentrates. Produced at mining facilities from various types of uranium-bearing ores and using various processes, uranium ore concentrates can consist of different uranium species, which provide an important clue when tracing interdicted samples back to their origins. The team reports the application of near-infrared spectroscopy as a noncontact, nondestructive method to rapidly analyze the concentrates for species or process information. Diffuse reflectance spectra from 350 to 2500 nm were measured from a number of samples, which were also characterized by x-ray diffraction and classified with principal component analysis.

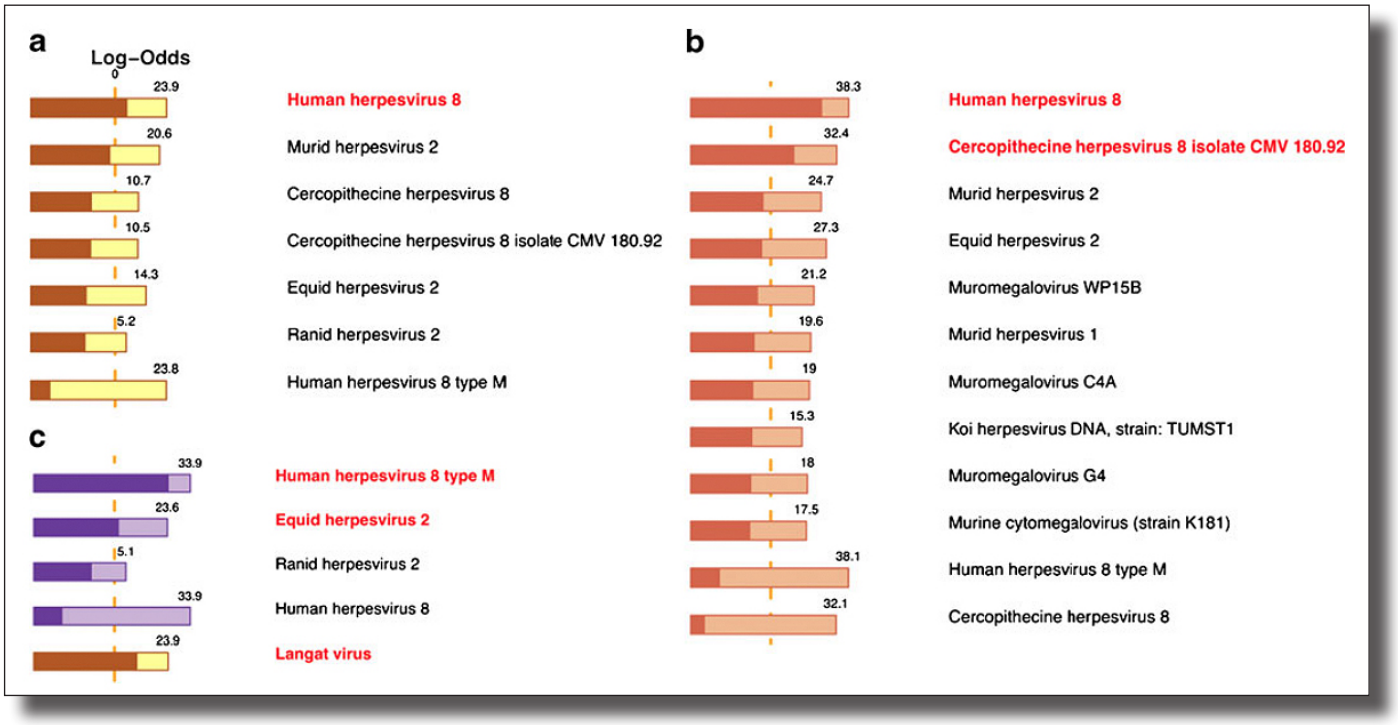


LIVERMORE RESEARCHERS—AND DETECTION ARRAY—IN MILESTONE BLADDER CANCER STUDY

Livermore biologist Crystal Jaing and computational biologist Kevin McLoughlin are coauthors on a paper published in *Tumor Biology* that **announces what is possibly the first-ever association between bladder cancer**—the seventh most common human malignancy—and Kaposi's sarcoma-associated herpesvirus, also known as human herpesvirus 8. In the study, the Lawrence Livermore Microbial Detection Array (LLMDA) was used in the initial screening of biopsy samples. The LLMDA version used covers all complete bacterial and viral genome sequences known as of early 2007 and revealed the presence of human herpesvirus 8, which was then verified with polymerase chain reaction. Said Crystal, "For us, it is the first publication showing the technology used as the primary detector of a virus associated with a specific disease, which was then confirmed using other techniques." The figure gives LLMDA analysis results for three biopsies (a through c), showing human herpesvirus 8 to be the most likely present among all target viruses.

ELEMENT 115 CONFIRMED

An international team of researchers, including some from LLNL, reported in *Physical Review Letters* that experiments conducted at the GSI Helmholtz Centre for Heavy Ion Research in Darmstadt, Germany, have **produced and detected element 115** (currently called ununpentium), thereby corroborating the first observation of the element in 2003 by a team of scientists from LLNL and Dubna, Russia. A committee from the International Union of Pure and Applied Chemistry (IUPAC), which governs chemical nomenclature, will review the new findings to decide whether more experiments are necessary before element 115 gets an official name. If approved by IUPAC, naming rights for the new element will go to the Dubna–LLNL team as the initial discoverers.

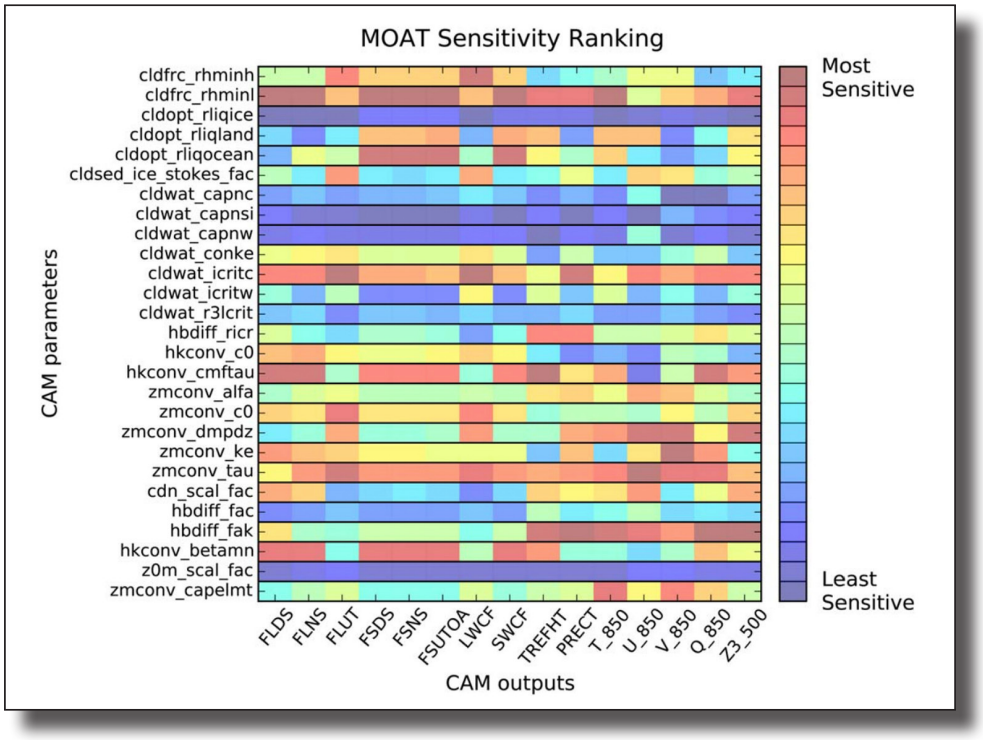


SUCCESS WITH NEW METHOD FOR ASSESSING CLIMATE-MODEL SENSITIVITY

In a paper published in *Journal of Advances in Modeling the Earth System*, Livermore's Curt Covey and colleagues **report their results using an algorithm for parameter-sensitivity screening**—the Morris one-at-a-time (MOAT) method—that drastically reduced the computational cost of estimating sensitivities in a high-dimensional parameter space. The team applied MOAT and traditional elementary one-at-a-time (EOAT) parameter variation to the Community Atmosphere Model (**CAM**), assessing CAM's behavior as a function of 27 input parameters. [The model output analyzed by the team was produced under the LDRD project "The Advance of Uncertainty Quantification Science" (**10-SI-013**).] For energy fluxes at the top of the atmosphere, EOAT and MOAT rank most input parameters similarly, but MOAT identified a sensitivity that EOAT underplays for two convection parameters that operate nonlinearly in the model. The figure is a MOAT ranking of 27 input parameters and shows, for instance, that nearly all are relatively sensitive to deep convection time scale (zmconv_tau) and minimum relative humidity for low cloud formation (cldfrc_rhminl).

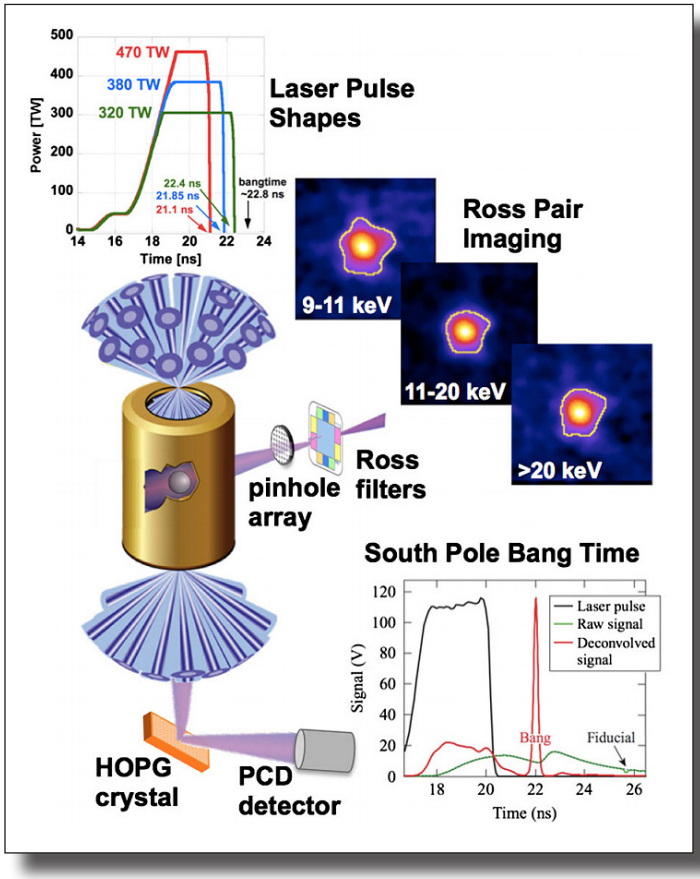
OZONE HOLE MAY CAUSE SLIGHT GLOBAL WARMING

Until now, the anthropogenic depletion of ozone in the Earth's stratosphere and severe seasonal depletion of ozone over the South Pole have been thought to induce cooling of the Earth, slightly offsetting the warming trend caused by greenhouse gasses. However, a new study published in *Geophysical Research Letters* suggests that **the ozone hole has a slight warming effect**. The influence is indirect and results from the hole's effect on winds: the shifting wind patterns caused by the ozone hole push clouds farther toward the South Pole, reducing the amount of solar radiation that clouds reflect and possibly causing a small amount of warming. The results are based on computer models of the coupled atmosphere–ocean system and are consistent with observations from the **International Satellite Cloud Climatology Project**, a decades-long NASA effort to map global cloud distributions. Mark Zelinka, of the Lab's **Program for Climate Model Diagnosis and Intercomparison**, co-authored the paper and participated in collaboration between Columbia University, NASA Goddard Institute for Space Studies, NYU, and LLNL. The Laboratory's participation was funded by the DOE's Office of Biological and Environmental Research.



NEW MODEL TO MEASURE HYDRODYNAMIC MIX IN FUSION IMPLOSIONS

A new model for **measuring the mix of ablator material into the hot spot** of a NIF inertial confinement fusion implosion was described in a *Physical Review Letters* paper by lead author Tammy Ma and colleagues at LLNL, Los Alamos, Rochester University, and General Atomics. The new model uses the ratio of experimentally measured x-ray emission to neutron yield to quantify the impurity mix of shell ablator into the hot spot. By applying this model to the full ensemble of NIF's cryogenically layered implosions, the researchers found that the high-velocity, high-convergence conditions in these experiments result in an increased hydrodynamic mix of the ablator into the hot spot. The results show that neutron yield and ion temperature drop as the hot-spot mix mass increases. The figure shows a target with an example of the laser pulse shapes used. Viewing the implosion through a diagnostic patch in the hohlraum, the Ross filters image the temperature- and density-sensitive x-ray emission.



INVESTIGATIONS OF MIX IN NIF IMPLOSIONS

A paper authored by Maria Alejandra Barrios-Garcia and her LLNL and Los Alamos colleagues and appearing in *Physics of Plasmas* **reports an analysis of gated x-ray implosion images** from more than 40 NIF shots conducted between 2010 and 2012. The shots included experiments using cryogenically layered deuterium–tritium and tritium–hydrogendeuterium fuel, as well as shots using gas-filled, plastic-shell symmetry capsules. The researchers used Fourier analysis of the images to quantify the evolution of "bright spots" in their hot-spot intensity profiles; the bright spots are caused by heterogeneous mixing of ablator material and fuel into the hot spot. Comparing the location of the bright spots with known isolated defects on the capsule surface, the researchers observed a strong correlation between bright-spot location and the fill tube used to inject fuel into the capsule. The results indicate that the fill tube is a significant "seed" for the ablation front instability, causing hot-spot mix. The fill tube is the predominant seed for symmetry capsules, while other capsule nonuniformities are dominant seeds for the cryogenically layered ice targets.

"LIFE THROUGH ICY IMPACTS" THEORY BOLSTERED

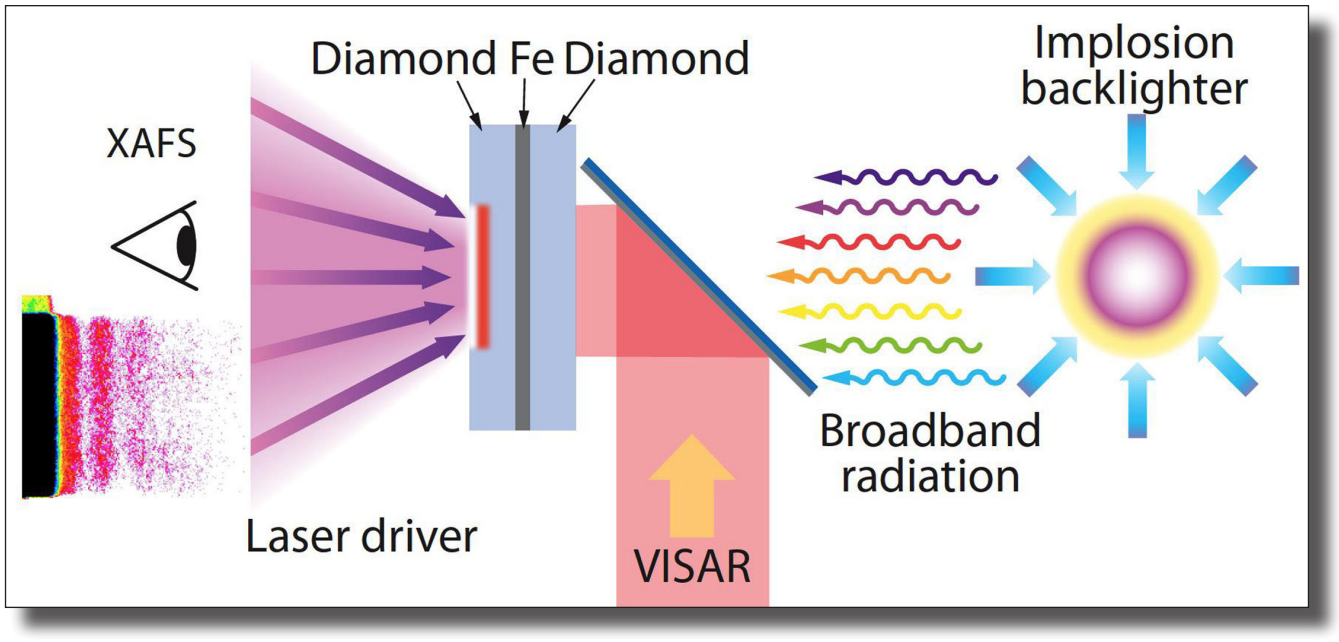
Livermore's Nir Goldman and colleagues from the U.K.'s Imperial College and University of Kent have published a paper in *Nature Geoscience* about laboratory experiments **suggesting that the impact on Earth of ancient comets** carrying simple substances such as methane could have been sufficient to produce the chemical precursors of life. (This publication follows on Nir's work being **featured on the cover** of *Journal of Physical Chemistry* earlier this year.) In the experiments, ice mixtures like those found in a comet were shocked with a gas gun. The results suggest that the hypervelocity impact shock of a comet containing a typical ice mixture could have indeed produced several kinds of amino acids. These findings thus suggest a potential pathway towards "life through icy impacts."

RECORD-SETTING IRON COMPRESSION IS ALSO EXAFS BREAKTHROUGH

In a series of campaigns led by the Laboratory's Yuan Ping and using the OMEGA laser at the University of Rochester, researchers compressed iron to pressures as great as 560 GPa (equivalent to 5.6 million times the pressure at the Earth's surface), a record pressure for solid iron. The team, **publishing in *Physical Review Letters***, achieved the pressure using multishock compression—a series of shocks rather than a single shock, thereby keeping entropy low while compressing the material—and verified the pressure using extended x-ray absorption fine structure (EXAFS) spectroscopy. This paper represents the first published data obtained with EXAFS for high-energy-density matter, a field where application of the powerful tool is still in its infancy. "Now," says Yuan, "the measurements can be scaled up to larger laser systems, such as the National Ignition Facility, to reach higher pressures or extended to shorter time scale to study dynamics in [high-energy-density] materials." Work at Livermore was supported by the LDRD Program. The figure shows the experimental setup used at the OMEGA laser, which diagnosed the properties of iron with extended x-ray absorption fine structure (XAFS), as well as a velocity interferometer system for any reflector (VISAR).

RECORD-SETTING EXPERIMENTS PROVIDE FIRST OBSERVATION OF MgO CRYSTALLINE PHASE

Researchers led by Livermore scientists Federica Coppari have found a new crystalline phase of magnesium oxide occurring above 600 GPa—"exoplanet pressures," **say the researchers in their paper in *Nature Geoscience***. Magnesium oxide is one of the main components of the Earth's mantle and of more massive exoplanets. Detailed knowledge of its structure and equation of state is of fundamental importance for understanding the formation and evolution of our planets as well as terrestrial exoplanets. In collaboration with Princeton University, the team used time-resolved x-ray diffraction techniques on the Omega laser to take a snapshot of the structure of magnesium oxide during dynamic compression, the first structural measurement of a structure that had been predicted by theoretical simulations. In this work, magnesium oxide had been ramp compressed to 900 GPa—the highest pressure at which x-ray diffraction data have ever been collected on any material. This work was supported by LLNL's Laboratory Directed Research and Development Program.

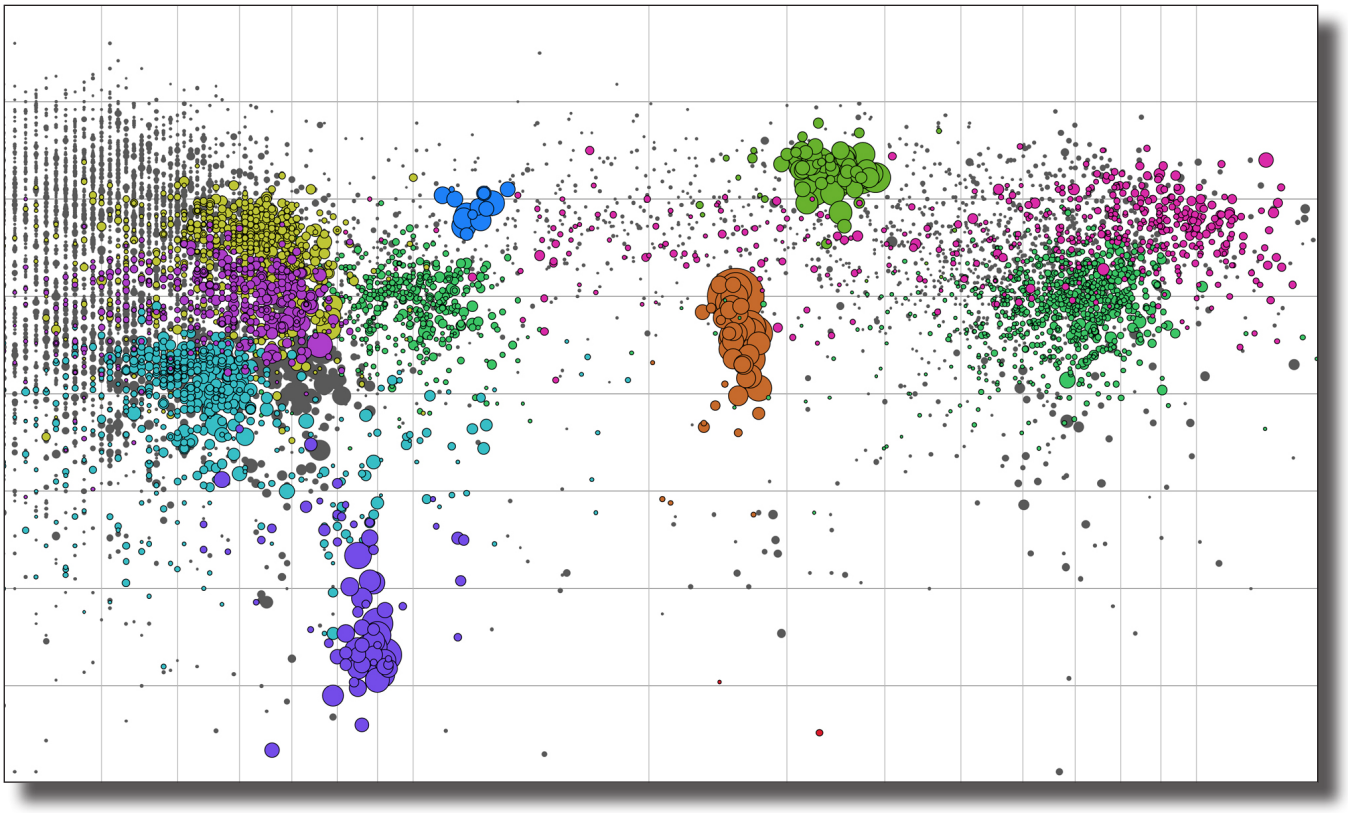


GENOMIC ADVANCE ANNOUNCED IN SWITCHGRASS BIOFUEL EXTRACTION

Publishing in *PLOS ONE*, a team including lead author Patrik D'haeseleer of LLNL and collaborators at the Joint Genome Institute and elsewhere **announced they have identified individual microbial species** whose enzymes are the most active in deconstructing switchgrass biomass in order to efficiently extract fermentable sugars for biofuel production. The researchers conducted metagenomic and proteogenomic analyses of a compost-derived bacterial consortium adapted to switchgrass and, for the first time, linked the functional roles of individual microbial populations within a consortium to specific enzyme activities. "Since these activities are broadly relevant to biofuel production," said co-author Steven Singer, of the Joint BioEnergy Institute, "this is one of the first real-world applications being met by combining metagenomics and metaproteomics." The figure is a splatterplot that visually represents the metagenome of the thermophilic bacterial consortium.

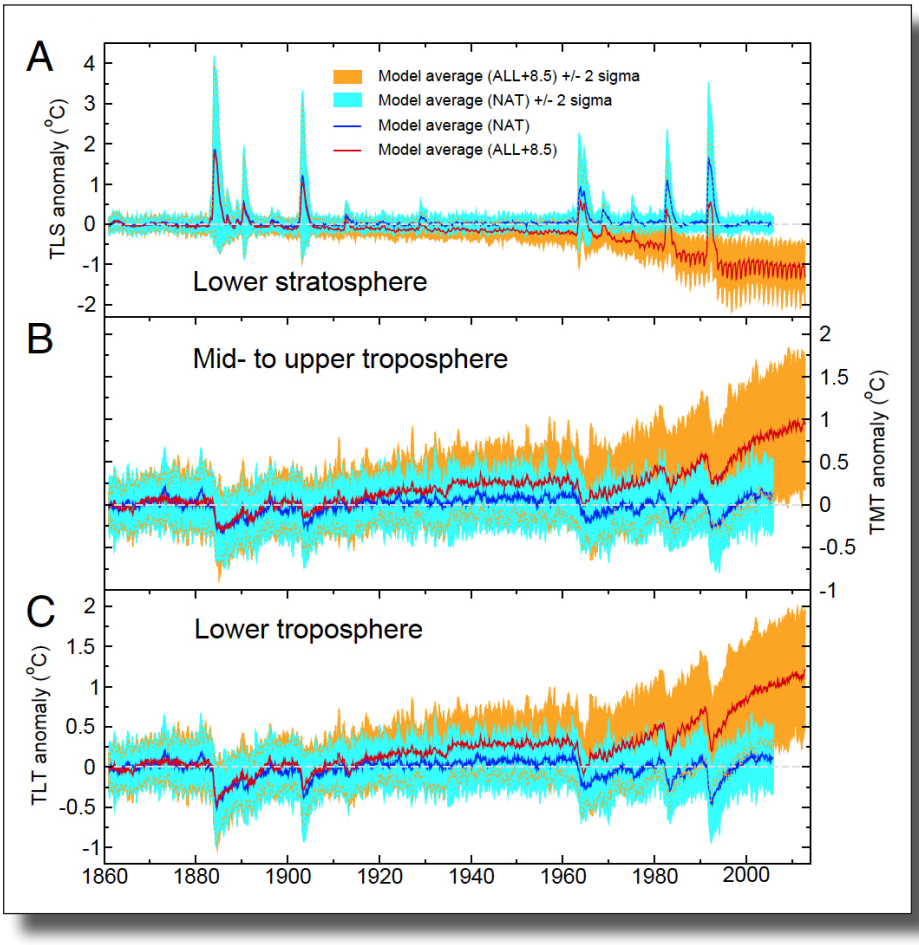
ALGORITHMIC BREAKTHROUGH FOR DISLOCATION DYNAMICS CALCULATIONS

LLNL material scientists Silvey Aubry and Tom Arsenlis, in a paper published in *Modeling and Simulation in Materials Science and Engineering*, **describe an analytical solution based on a spherical harmonics expansion** for calculating the interaction force between two dislocation segments in anisotropic elastic media. Compared to previous numerical methods, this new formulation is between 10 and 10,000 times faster, depending on the position of two segments. Using this new method, it is now practical to model anisotropic elasticity using dislocation dynamics, which will enable dislocation dynamics researchers to answer important questions about the behavior, motion, and interactions of dislocations in crystals that could not be accurately answered before. For instance, it will be possible to predict how a crystalline material will change in strength at extreme temperatures and pressures—conditions in which elastic anisotropy has been found to be greatest.



PAPER IN *PNAS* DESCRIBES HUMAN IMPACT ON ATMOSPHERIC TEMPERATURES

A multi-institutional team led by Benjamin Santer published in the *Proceedings of the National Academy of Sciences* **findings that human influences have directly impacted** the latitude and altitude pattern of atmospheric temperature. The research, which compares multiple satellite records of atmospheric temperature change with results from a large, multimodel archive of simulation, reveals global-scale tropospheric warming and stratospheric cooling over the 34-year satellite temperature record. Says Ben: "The pattern of temperature change that has been observed vertically in the atmosphere, from ground level to the stratosphere, fits with what is expected from human-caused increases in greenhouse gases. The observed pattern conflicts with what would be expected from an alternative explanation, such as fluctuations in the sun's output." In the figure are time series of temperature anomalies in the lower stratosphere (TLS), mid- to upper troposphere (TMT), and lower troposphere (TLT) (A through C, respectively).

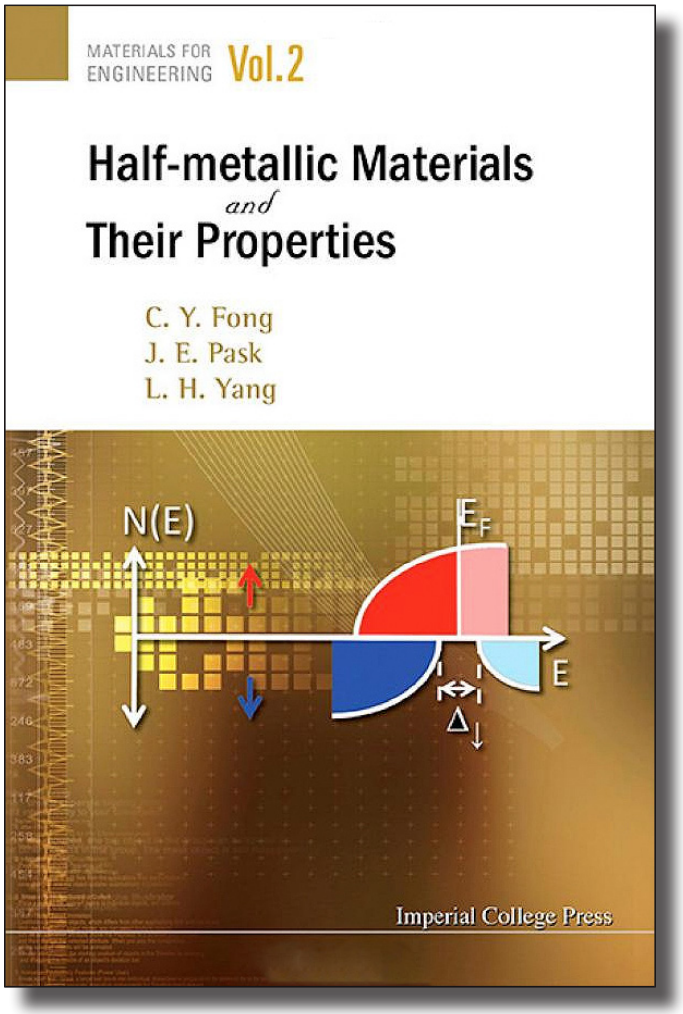


NUCLEAR DIAGNOSTICS AT NIF HELP UNRAVEL SIX-DECADE-OLD MYSTERY ABOUT TRITIUM–TRITIUM REACTION

Despite six decades of laboratory investigations, much uncertainty remains about the energy distribution of neutrons produced by the fusion of two tritium nuclei. In a recent paper published in *Physical Review Letters*, Livermore postdoc Daniel Sayer and colleagues **present neutron time-of-flight spectra from inertial confinement fusion experiments** with tritium-filled targets at NIF. Improvements in the diagnostics have resulted in a significant improvement in energy resolution and statistics over previous measurements, and allow the first definitive observation of a peak resulting from sequential decay through the ground state of ^{5}He at low reaction energies. The paper also demonstrates the importance of quantum interferences in interpreting the spectrum, which result from fermion symmetry between the two neutrons emitted from the reaction and the different decay channels. The neutron spectrum and analysis provide a better understanding of the conditions created in inertial confinement fusion implosions at NIF. This work was a collaborative effort among many LLNL scientists and their colleagues at Ohio University, the University of Rochester, Indiana University, MIT, LANL, and General Atomics.

RESEARCHERS PUBLISH BOOK ON HALF-METALS

Livermore's John Pask and Lin Yang, along with C. Y. Fong of UC Davis, have released *Half-Metallic Materials and Their Properties*, the first **comprehensive book on these materials**, which act as a conductor to electrons having one spin orientation but as an insulator or semiconductor to electrons with the opposite spin orientation. The book provides a detailed treatment of half-metallic materials and their properties from both an experimental and theoretical point of view, discusses the methods used to understand and predict the properties of half-metals and the many other materials to which these techniques are applicable, and also offers an expansive bibliography to facilitate further and deeper research.



REVELATION ON NIF HOT-SPOT MIXING IN PRL

A *Physical Review Letters* paper addressing a cause of problematic hot-spot cooling in NIF ignition experiments **presents the first experimental evidence** that hot-spot mix—that is, the mixing of plastic ablator material deep into the hot spot of ignition-scale fusion implosions—is caused primarily by ablation-front instability. The paper also provides a quantitative estimate of the amount of ablator mass mixed into the hot spot. The researchers used x-ray spectroscopy to study hot-spot mixing of plastic ablator material doped with copper and germanium placed at different radial locations in the ablator. They concluded that ablation-front hydrodynamic instabilities seeded by high-mode ablator-surface mass perturbations from intrinsic capsule surface roughness, the fill tube, or microscopic dust particles can mix ablator material into the interior of the deuterium–tritium fuel layer if the initial amplitudes and growth during the acceleration phase are large enough. Strategies to control hot-spot mix from the ablation-front instability, the researchers said, include reducing the capsule surface-mass perturbations, reducing the growth factors of the hydrodynamic instability, or changing to another ablator material such as copper-doped beryllium.

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